Perancangan Proses Kimia

PERANCANGAN SISTEM/JARINGAN REAKTOR

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Rancangan Kuliah Section 2

1. Dasar-dasar Penggunaan CHEMCAD/HYSYS
2. **Perancangan Sistem/jaringan Reaktor**
3. Tugas 1 dan Pembahasannya
4. Perancangan Sistem/jaringan Pemanas
5. Perancangan Sistem/jaringan Separator & Recycle
6. Tugas 2 dan Pembahasannya
7. Studi Kasus
8. Ujian Section 2

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Chemical Reactor Models

- Chemical Reactors are designated to involve:
  - multiple phases (vapor, liquid, reacting solid, solid catalyst)
  - different geometris (stirred tank, tubular flows, converging and diverging nozzles, spiral flows, and membrane transport)
  - various regimes of momentum, heat and mass transfer (viscous flow, turbulent flow, conduction, radiation, diffusion, and dispersion)

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Types of Reactor Models in Simulator

- **Stoichiometric Reactor** (permits the specification of reactant conversion and extents of reaction for one or more specified reactions)
- **Equilibrium Reactor** (model for multiple phases (vapor, liquid, solid) in chemical equilibrium)
- **Kinetic Reactor** (CSTR & Plug Flow)
- **Gibbs Reactor** (for mass and energy balance, no stoichiometric reaction required)

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Stoichiometric Reactor

- Digunakan untuk mensimulasikan:
  - Reaksi tunggal dengan satu set koefisien reaksi
  - Komponen kunci dan konversi diketahui
  - Reaksi dapat berlangsung secara adiabatik, isotermik, atau dengan pengeluaran/pemasukan panas
- Masukkan faktor-faktor stoikiometri reaksi, negatif bila reaktan, dan positif bila produk, dan nol bila tidak bereaksi

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Reaction Stoichiometry

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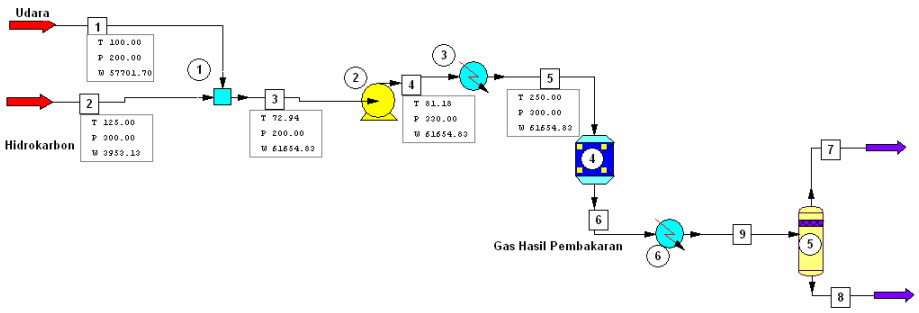

Stream No.	1	2	3	4	5	6
Name	Udara	Fuel	Keluar Mixer	Masuk HE	Masuk Reakto	Hasil Pembak
- - Overall - -						
Molar flow lbmol/h	2000.0000	100.0000	2100.0000	2100.0000	2100.0000	2167.5000
Mass flow lb/h	57701.7031	3953.1250	61654.8281	61654.8281	61654.8281	61654.7578
Temp F	100.0000	125.0000	72.9361	81.1836	250.0000	3070.4230
Pres psia	200.0000	300.0000	200.0000	330.0000	300.0000	300.0000
Vapor mole fraction	1.000	0.5662	1.000	1.000	1.000	1.000
Enth MMBtu/h	0.25119	-1.3749	-1.1237	-1.0534	1.7351	1.7351
Flowrates in lb/h						
Nitrogen	44262.1211	0.0000	44262.1211	44262.1211	44262.1211	44262.1211
Oxygen	13439.5801	0.0000	13439.5801	13439.5801	13439.5801	3719.8838
3-Mth-1-Pentene	0.0000	3787.2451	3787.2451	3787.2451	3787.2451	946.8113
Helium-3	0.0000	165.8800	165.8800	165.8800	165.8800	165.8800
Water	0.0000	0.0000	0.0000	0.0000	0.0000	3648.0374
Carbon Dioxide	0.0000	0.0000	0.0000	0.0000	0.0000	8912.0244

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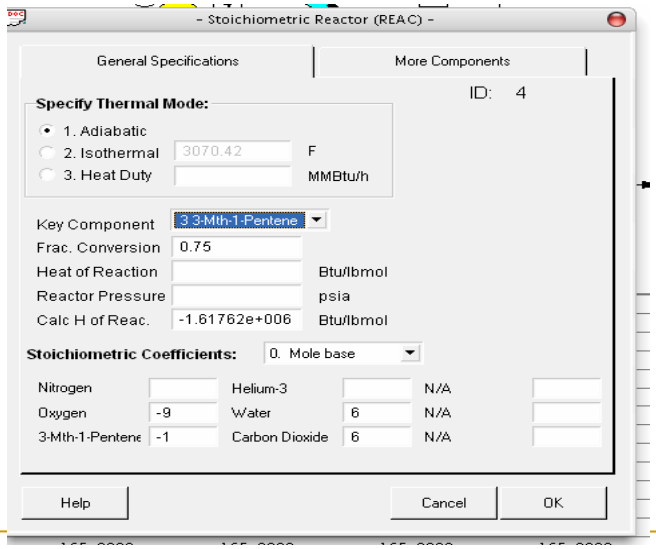
Setting Stoichiometric Reactor



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Equilibrium Reactor

- Digunakan untuk mensimulasikan:
  - Lebih dari 20 reaksi simultan
  - Reaksi-reaksi tersebut diketahui konversinya atau rasio kesetimbangan
  - Masing-masing reaksi dapat mengandung lebih dari 10 komponen
  - Laju alir produk, komposisi, dan kondisi termal dapat dihitung melalui persamaan kesetimbangan reaksi
  - Reaksi fasa cair maupun fasa uap
  - Reaksi dapat isotermal atau adiabatik

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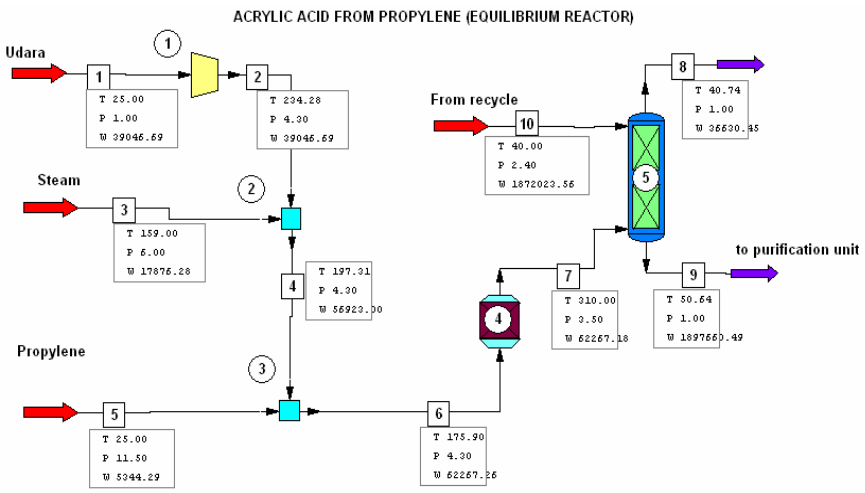
Example: Equilibrium Reactor



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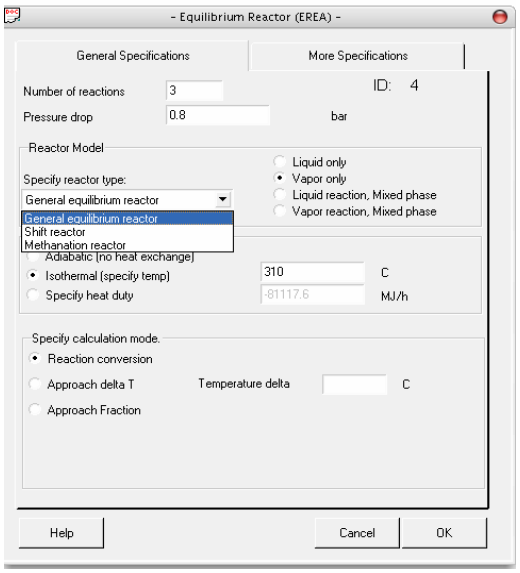

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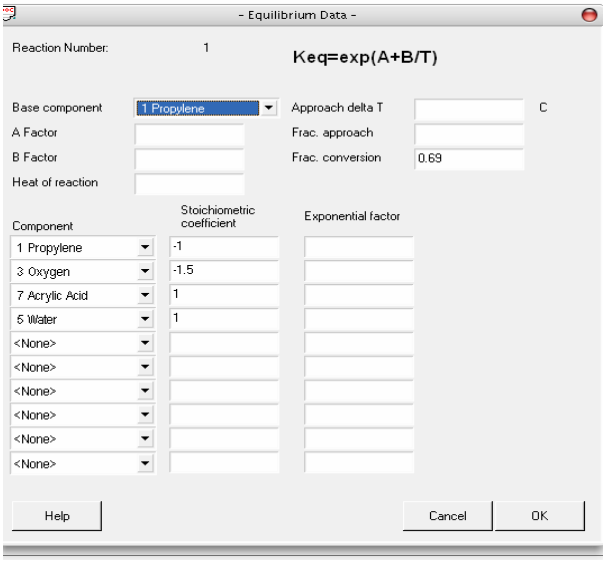
- Equilibrium Data -
Reaction Number: 1
Keq=exp(A+B/T)
Base component 1 Propylene
A Factor
B Factor
Heat of reaction
Approach delta T
Frac. approach
Frac. conversion 0.69
C
Component
Stoichiometric coefficient
Exponential factor
1 Propylene -1
3 Oxygen -1.5
7 Acrylic Acid 1
5 Water 1
<None>
Help
Cancel
OK

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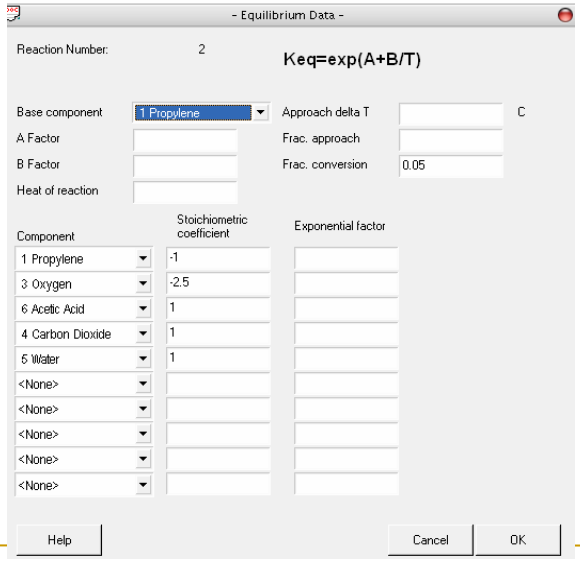
- Equilibrium Data -
Reaction Number: 2
Keq=exp(A+B/T)
Base component 1 Propylene
A Factor
B Factor
Heat of reaction
Approach delta T
Frac. approach
Frac. conversion 0.05
C
Component
Stoichiometric coefficient
Exponential factor
1 Propylene -1
3 Oxygen -2.5
6 Acetic Acid 1
4 Carbon Dioxide 1
5 Water 1
<None>
Help
Cancel
OK

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Kinetic Reactor

- Reaktor ini dapat digunakan untuk mensimulasikan:
  - Plug Flow Reactor (PFR) dan Continuous Stirred Tank Reactor (CSTR)
  - Lebih dari 20 reaksi simultan
  - Konversi total komponen kunci diketahui dan akan dihitung volume reaktornya atau kebalikannya
  - Reaksi fasa uap, cair, atau campuran
  - Reaksi-reaksi yang diketahui data-data kinetikanya (faktor frekuensi, energi aktivasi, faktor eksponensial, faktor adsorpsi, energi adsorpsi, etc.)
  - Laju kinetika dapat dibuat standar atau dispesifikasikan oleh pengguna
  - Reaksi dapat bersifat adiabatik atau isotermal

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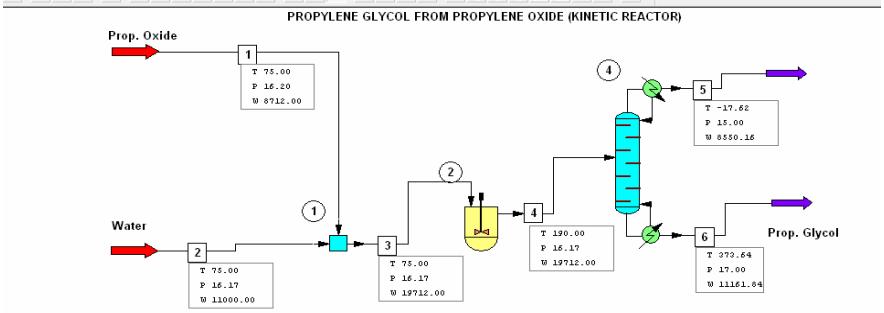
Example: Kinetic Reactor



Stream No.	1	2	3	4	5	6
Name	Prop. Oxide	Water				
- - Overall - -						
Molar flow lbmol/h	150.0000	610.6023	760.6023	614.0511	466.8061	147.2449
Mass flow lb/h	8712.0000	11000.0000	19712.0000	19712.0020	8550.1631	11161.8379
Temp F	75.0000	75.0000	74.9994	190.0000	-17.6243	373.6404
Pres psia	16.2000	16.1700	16.1700	16.1700	15.0000	17.0000
Vapor mole fraction	0.0000	0.0000	0.0000	0.003809	0.0000	0.0000
Enth MMBtu/h	-7.8119	-75.020	-82.832	-86.136	-57.901	-28.474
Actual vol ft3/hr	169.2217	176.7366	345.9582	1316.7881	137.3948	202.5250
Std liq ft3/hr	167.1261	176.2315	343.3576	309.1785	137.6139	171.5646
Std vap 60F scfh	56921.7930	231710.5156	288632.3125	233019.2813	177142.9219	55876.2930
Flowrates in lbmol/h						
1-2-Propylene Ox	150.0000	0.0000	150.0000	3.4488	3.4488	0.0000
1-2-Propanediol	0.0000	0.0000	0.0000	146.5512	0.0426	146.5086
Water	0.0000	610.6023	610.6023	464.0511	463.3146	0.7363

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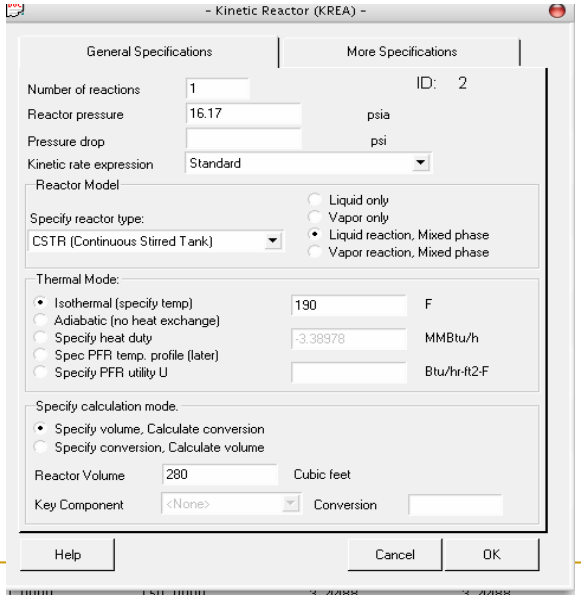

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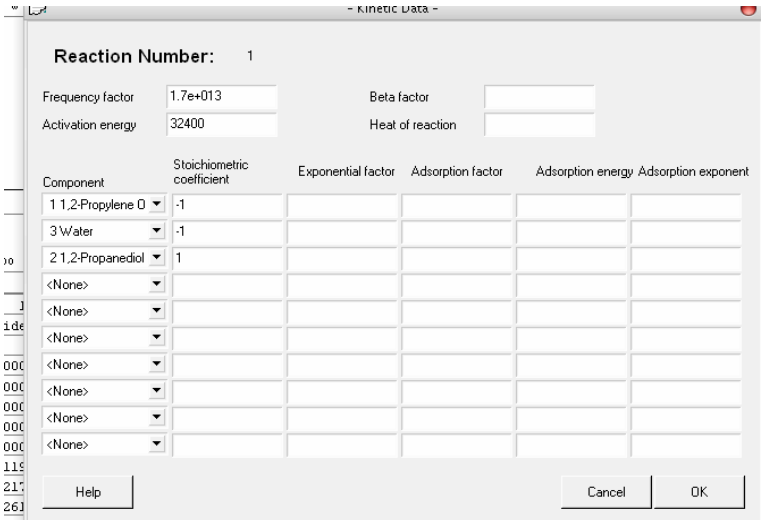

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Gibbs Reactor

- Reaktor ini dapat digunakan untuk mensimulasikan:
  - tujuan neraca massa dan energi
  - tidak memerlukan stoikiometri
  - Laju alir produk, komposisi, kondisi termal dihitung dengan meminimasi energi bebas Gibbs, cenderung kepada neraca massa keseluruhan
  - Reaktor dapat dioperasikan dengan fasa tunggal (cair atau uap) atau campuran
  - dapat dioperasikan secara isotermal
  - komponen inert dapat dispesifikasi

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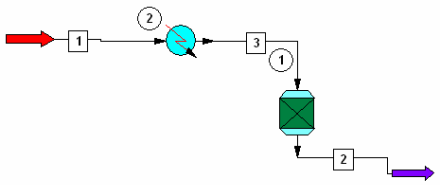
Example: Gibbs Reactor

Gibbs Reactor (Minimization of Gibbs Free Energy)



Stream No.	1	2
Name	FEED	PRODUCT
- - Overall - -		
Molar flow kmol/h	10.0723	17.1841
Mass flow kg/h	220.0000	219.9956
Temp C	100.0000	800.0000
Pres atm	5.0000	4.9000
Vapor mole fraction	1.000	0.9522
Enth MJ/h	-441.04	-2023.3
Flowrates in kmol/h		
Methane	6.2332	1.1148
Hydrogen	0.0000	8.8809
Carbon Monoxide	0.0000	3.7016
Nitrogen	0.7139	0.7139
Oxygen	3.1251	0.0000
Water	0.0000	1.3561
Carbon Dioxide	0.0000	0.5962
Carbon	0.0000	0.8206

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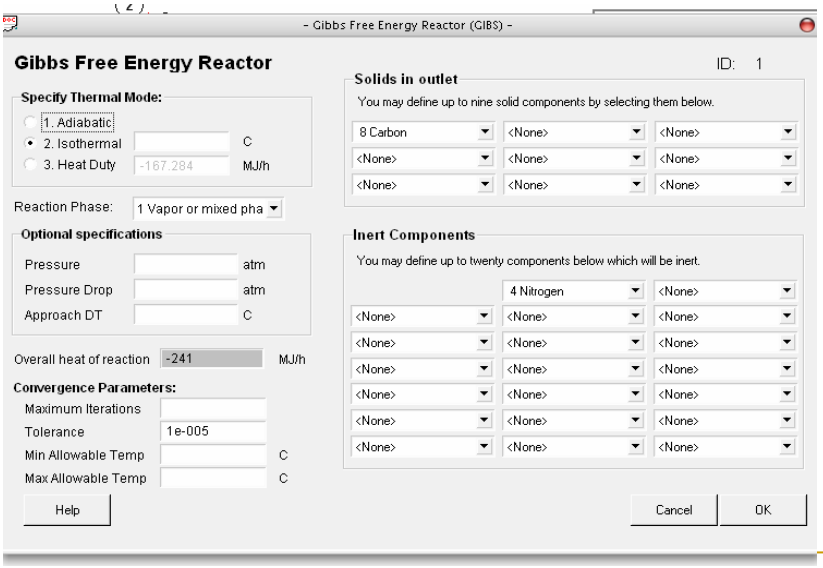
- Gibbs Free Energy Reactor (GIBS) -
Gibbs Free Energy Reactor
ID: 1
Specify Thermal Mode:
1. Adiabatic
2. Isothermal
C
3. Heat Duty
-167.284
MJ/h
Reaction Phase:
1 Vapor or mixed pha
Optional specifications
Pressure
atm
Pressure Drop
atm
Approach DT
C
Overall heat of reaction
-241
MJ/h
Convergence Parameters:
Maximum Iterations
Tolerance
1e-005
Min Allowable Temp
C
Max Allowable Temp
C
Help
Solids in outlet
You may define up to nine solid components by selecting them below.
8 Carbon
<None>
Inert Components
You may define up to twenty components below which will be inert.
4 Nitrogen
Cancel
OK

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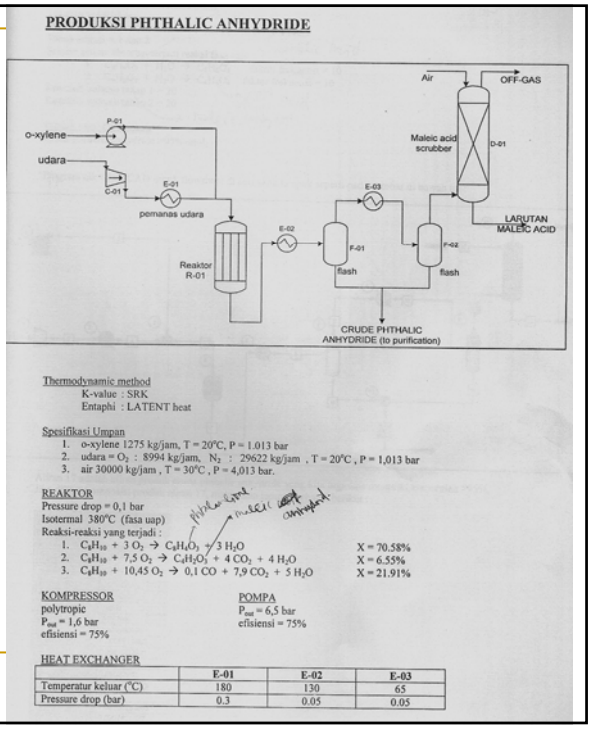
TUGAS 1


PRODUKSI PHTHALIC ANHYDRIDE
o-xylene
udara
P-01
C-01
E-01
pemanas udara
Reaktor R-01
E-02
E-03
F-01
flash
F-02
flash
Air
OFF-GAS
Maleic acid scrubber
D-01
LARUTAN MALEIC ACID
CRUDE PHTHALIC ANHYDRIDE (to purification)
Thermodynamic method
K-value : SRK
Entaphi : LATENT heat
Spesifikasi Umpan
1. o-xylene 1275 kg/jam, T = 20°C, P = 1.013 bar
2. udara = O2 : 8994 kg/jam, N2 : 29622 kg/jam , T = 20°C , P = 1,013 bar
3. air 30000 kg/jam , T = 30°C , P = 4,013 bar.
REAKTOR
Pressure drop = 0,1 bar
Isotermal 380°C (fasa uap)
Reaksi-reaksi yang terjadi :
1. C8H10 + 3 O2 → C8H4O3 + 3 H2O X = 70.58%
2. C8H10 + 7,5 O2 → C4H2O3 + 4 CO2 + 4 H2O X = 6.55%
3. C8H10 + 10,45 O2 → 0,1 CO + 7,9 CO2 + 5 H2O X = 21.91%
KOMPRESSOR
polytropic
Pout = 1,6 bar
efisiensi = 75%
POMPA
Pout = 6,5 bar
efisiensi = 75%
HEAT EXCHANGER
E-01 E-02 E-03
Temperatur keluar (°C) 180 130 65
Pressure drop (bar) 0.3 0.05 0.05